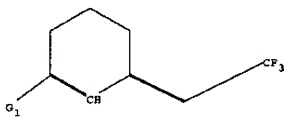
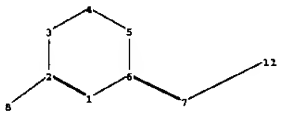
C:\STNEXP4\QUERIES\285937f3.str

12-16-03



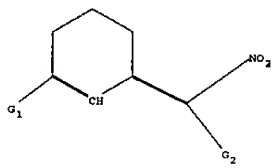

chain nodes :
7 8 11
ring nodes :
1 2 3 4 5 6
chain bonds :
2-8 6-7 7-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 4-5 5-6
exact bonds :
6-7 7-11

G1:C,H,O,S,N,P

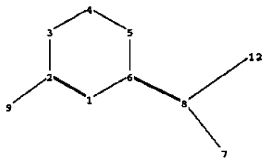
G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS

C:\STNEXP4\QUERIES\285937m.str




No answer for the present application



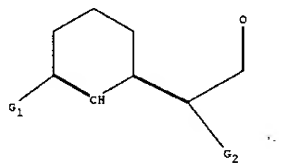

chain nodes :
7 8 9 12
ring nodes :
1 2 3 4 5 6
chain bonds :
2-9 6-8 7-8 8-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-8
exact bonds :
6-8 8-12

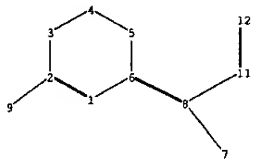
G1:C,H,O,S,N,P

G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS

C:\STNEXP4\QUERIES\285937m.str




chain nodes :
7 8 9 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
2-9 6-8 7-8 8-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-8 11-12
exact bonds :
6-8 8-11

G1:C,H,O,S,N,P

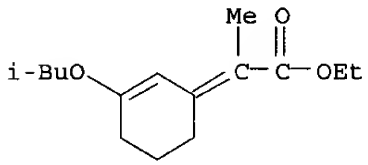
G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS

RN 14736-74-4 REGISTRY
CN 2-Cyclohexene-.DELTA.1,.alpha.-acetic acid, 3-isobutoxy-.alpha.-methyl-, ethyl ester (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |




Calculated Properties (CALC)

| CODE | PROPERTY | VALUE | CONDITION | NOTE |
|---|---|---|---|---|
| HD | H donors | 0 | | ACD (1) |
| HAC | H acceptors | 3 | | ACD (1) |
| MW | Molecular Weight | 252.35 | | ACD (1) |
| LOGP | logP | 4.217+/-0.362 | | ACD (1) |
| FRB | Freely Rotatable Bonds | 6 | | ACD (1) |
| LOGD | logD | 4.22 | pH 1 | ACD (1) |
| LOGD | logD | 4.22 | pH 4 | ACD (1) |
| LOGD | logD | 4.22 | pH 7 | ACD (1) |
| LOGD | logD | 4.22 | pH 8 | ACD (1) |
| LOGD | logD | 4.22 | pH 10 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 1 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 4 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 7 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 8 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 10 | ACD (1) |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 67:2802 CA
TI Synthesis of cyclohexane derivatives
AU Tanaka, Tsuguo
CS Univ. Saga, Saga, Japan
SO Bull. Chem. Soc. Jpn. (1967), 40(1), 233-4
CODEN: BCSJA8
DT Journal
LA English

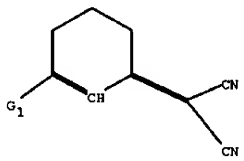
CC 24 (Alicyclic Compounds)

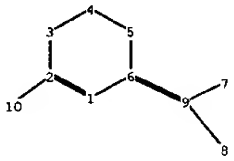
AB The synthesis of cyclohexane derivs. by means of the Michael condensation of 2 appropriate cyclohexane derivs. was described. Dihydroresorcinol was treated with iso-BuOH and p-toluenesulfonic acid to give an 89% yield of its isobutyl enol ether, b3 101-3.degree., which was treated with Zn and Et .alpha.-bromopropionate at 120.degree. (Reformatsky reaction) to give 50% of a product, b3 99-101.degree.. This product was hydrolyzed with HCl to give a conjugate enone, 3-(.alpha.-carbethoxyethyl)-2-cyclohexen-1-one (I), b4 123-7.degree.. The 2,4-dinitrophenylhydrazone deriv. of I was hydrogenated over 5% Pd-charcoal to give an 82.5% yield of a satd. ketone, 3-(.alpha.-carbethoxyethyl)cyclohexan-1-one (II), b3.5 111-12.degree.. The cyanohydrin of II, prepd. by treating II with HCN, was dehydrated with SOCl2 in a pyridine soln. at room temp. overnight. The product (44.5% yield, b3 126.5-8.5) was sepd. by vapor-phase chromatog. into 1-cyano-3-(.alpha.-carbethoxyethyl)cyclohexene and 1-cyano-5-(.alpha.-carbethoxyethyl)cyclohexene. Dimethyldihydroresorcinol was treated with HCO2Et and Na methoxide in a C6H6 soln. overnight to give a 24% yield of 2,2-dimethyl-4 - hydroxymethylenecyclohexanedione 1,3 - monoethylene ketal, b4 106.0-10.5.degree..

ST CYCLOHEXENES; CYCLOHEXENONES; RESORCINOLS DIHYDRO

IT 14736-74-4P 14736-75-5P 14736-76-6P 14736-77-7P 14736-78-8P
14736-79-9P 14736-80-2P 14736-81-3P 14736-82-4P 14782-52-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

C:\STNEXP4\QUERIES\285937.str




chain nodes :
7 8 9 10
ring nodes :
1 2 3 4 5 6
chain bonds :
2-10 6-9 7-9 8-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-10 3-4 4-5 5-6
exact bonds :
6-9 7-9 8-9

G1:C,H,O

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS

AN 1992:407540 CAPLUS
DN 117:7540
ED Entered STN: 11 Jul 1992
TI Reactions of trifluoromethyl ketones. VIII. Investigation of steric effect of a trifluoromethyl group through ene reaction of trifluoromethyl ketones
AU Nagai, Takabumi; Nishioka, Goro; Koyama, Mayumi; Ando, Akira; Miki, Takuichi; Kumadaki, Itsumaro
CS Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01, Japan
SO Chemical & Pharmaceutical Bulletin (1992), 40(3), 593-8
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 22
OS CASREACT 117:7540
AB In the ene reaction of trifluoromethyl ketones, a trifluoromethyl group has been obsd. to behave as a larger substituent than commonly believed in the biomedicinal field. To est. the steric effect of a trifluoromethyl group, several trifluoromethyl ketones RCOCF3 (R = H, Me, Bu, Ph, Me2CHCH2, cyclohexyl, EtMeCH, CF3, thexyl) were prepd. and their ene reaction with cyclohexene, a 1,2-disubstituted ene having the least steric requirement, examd. In this reaction, a trifluoromethyl group was found to behave as if it were a much larger substituent than a Ph or iso-Bu group and as large as a sec-Bu group.
ST steric effect trifluoromethyl group ene reaction; ketone trifluoromethyl ene reaction; stereochem ene reaction trifluoromethyl ketone; regiochem ene reaction trifluoromethyl ketone
IT Steric effect
(of trifluoromethyl group on ene reaction of trifluoromethyl ketones)
IT Trifluoromethyl group
(steric effect of, on ene reactions of trifluoromethyl ketones)
IT Addition reaction
(ene, of trifluoromethyl ketones, steric effect of trifluoromethyl group on)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(trifluoromethyl, ene reaction of, steric effect of trifluoromethyl group on)
IT 76-05-1, Trifluoroacetic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of)
IT 108-85-0, Cyclohexyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with iso-Bu trifluoromethyl ketone)
IT 78-77-3, Isobutyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetic acid)
IT 1521-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetophenone)
IT 75-90-1, Trifluoroacetaldehyde 360-34-9 421-50-1 434-45-7, .alpha.,.alpha.,.alpha.-Trifluoroacetophenone 684-16-2, Hexafluoroacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, steric effect of the trifluoromethyl group in)
IT 433-27-2, Trifluoroacetaldehyde ethyl hemiacetal
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with dimethylbutenes)
IT 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with trifluoroacetaldehyde)
IT 110-83-8, Cyclohexene, reactions 13389-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with trifluoromethyl ketones)

IT 116356-54-8P 122129-36-6P 122129-38-8P 141779-27-3P 141779-28-4P
141779-29-5P 141779-30-8P 141779-31-9P **141779-32-0P**
141779-33-1P **141779-34-2P 141779-35-3P** 141779-36-4P
**141779-37-5P 141779-38-6P 141779-39-7P**
141779-42-2P 141779-43-3P 141779-44-4P 141846-75-5P 141846-76-6P
141846-77-7P 141899-03-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)

IT 114420-54-1P 122129-28-6P 122129-29-7P 122129-30-0P 122129-31-1P
125458-29-9P 134166-51-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 134166-52-2P 134166-53-3P 134166-54-4P 134166-55-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and dehydration of)

IT 6302-04-1P, Cyclohexyl trifluoromethyl ketone 75703-02-5P, Isobutyl trifluoromethyl ketone 134166-49-7P, sec-Butyl trifluoromethyl ketone 134166-50-0P, Thexyl trifluoromethyl ketone
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and ene reaction of, steric effect of the trifluoromethyl group in)

IT 141779-40-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and hydrogenation of)

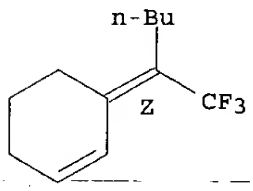
IT 141779-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and oxidn. of)

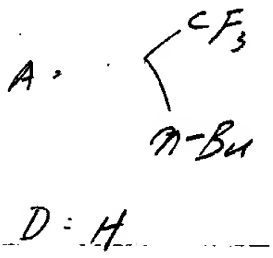
IT **141779-32-0P 141779-34-2P 141779-35-3P**
**141779-37-5P 141779-38-6P 141779-39-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)

RN 141779-32-0 CAPLUS

CN Cyclohexene, 3-[1-(trifluoromethyl)pentylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

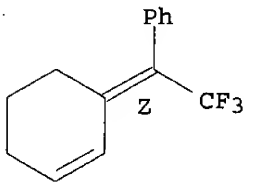


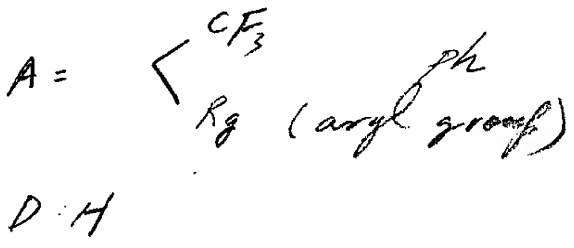




RN 141779-34-2 CAPLUS

CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



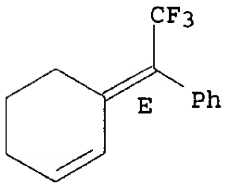




RN 141779-35-3 CAPLUS

CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (E)- (9CI)

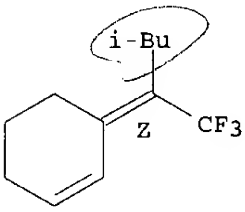
(CA INDEX NAME)

Double bond geometry as shown.



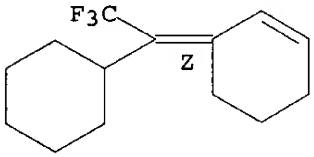

RN 141779-37-5 CAPLUS
CN Cyclohexene, 3-[3-methyl-1-(trifluoromethyl)butylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



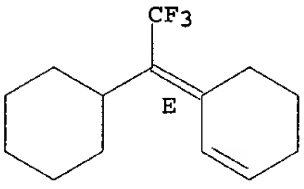

RN 141779-38-6 CAPLUS
CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.




RN 141779-39-7 CAPLUS
CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (E)- (9CI) (CA INDEX NAME)

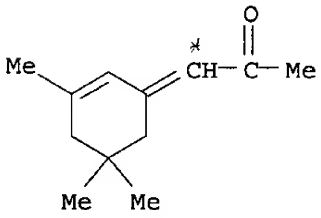
Double bond geometry as shown.



RN 3211-80-1 REGISTRY
CN 2-Propanone, 1-(3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Propanone, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (7CI, 8CI)
FS 3D CONCORD
DR 178117-22-1
MF C12 H18 O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMLIST, TOXCENTER
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |




$R_1$ : H  $R_{m,n,\beta,\gamma}$ : H

$R_A$ : $CH_3$

D : $CH_3$

$R_o$ & $R_p$ : $CH_3$

Calculated Properties (CALC)

| CODE | PROPERTY | VALUE | CONDITION | NOTE |
|---|---|---|---|---|
| HD | H donors | 0 | | ACD (1) |
| HAC | H acceptors | 1 | | ACD (1) |
| MW | Molecular Weight | 178.27 | | ACD (1) |
| LOGP | logP | 3.334+/-0.241 | | ACD (1) |
| FRB | Freely Rotatable Bonds | 1 | | ACD (1) |
| LOGD | logD | 3.33 | pH 1 | ACD (1) |
| LOGD | logD | 3.33 | pH 4 | ACD (1) |
| LOGD | logD | 3.33 | pH 7 | ACD (1) |
| LOGD | logD | 3.33 | pH 8 | ACD (1) |
| LOGD | logD | 3.33 | pH 10 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 1 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 4 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 7 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 8 | ACD (1) |
| SLB.MOL | Molar Solubility | <0.01 mol/L | pH 10 | ACD (1) |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1

AN 129:44683 CA
TI Evaluation of organic pollutants in a contaminated area
AU Rotatori, Mauro; Bertoni, Giuliano; Ferragina, Carla; Maio, Giovanni; Tappa, Remo
CS Istituto sull'Inquinamento Atmosferico, Montelibretti, C.N.R., Rome, Italy
SO Acqua Aria (1998), (3), 109-117
CODEN: AQARDW; ISSN: 0391-5557
PB Arti Poligrafiche Europee Srl
DT Journal
LA Italian
CC 60-6 (Waste Treatment and Disposal)
Section cross-reference(s): 19, 80
AB A sampling-anal. strategy for contaminated soils which permits to collect a large amt. of quant. and qual. data in a reasonably short time is proposed. Various anal. techniques: thermal desorption-gas chromatog. anal. (TF-GC), solvent extn. followed by gas chromatog./mass-spectrometric anal. (GC-MS), thermogravimetry with DTA (TG-DTA) and powder diffractometry (XRPD) were used and compared in order to characterize samples of soils. Results of a study performed in an industrial area contaminated by unknown org. compds. were obtained. About 70 org. pollutants were identified. The vertical distribution profile of org. pollutants is discussed.
ST org pollutant contaminated soil analysis
IT Soils
(contaminated; org. pollutant detn. in contaminated soils)
IT Sampling
(org. pollutant detn. in contaminated soils)
IT Organic compounds, analysis
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)
(org. pollutant detn. in contaminated soils)
IT 50-32-8, Benzo[a]pyrene, analysis 78-59-1 84-66-2, 1,2-Benzenedicarboxylic acid, diethyl ester 84-69-5, 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester 85-01-8, Phenanthrene, analysis 88-69-7 91-20-3, Naphthalene, analysis 95-63-6, 1,2,4-Trimethylbenzene 98-82-8, 1-Methylethylbenzene 99-87-6, 1-MEthyl-4-(1-methylethyl)-benzene 100-51-6, Benzenemethanol, analysis 100-52-7, Benzaldehyde, analysis 100-53-8, Benzenemethanethiol 103-29-7 103-65-1, Propylbenzene 108-10-1, 4-Methyl-2-pentanone 111-82-0, Dodecanoic acid, methyl ester 111-84-2, Nonane 112-40-3, Dodecane 117-81-7, 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester 120-61-6, 1,4-Benzenedicarboxylic acid, dimethyl ester 122-57-6 123-42-2 124-18-5, Decane 129-00-0, Pyrene, analysis 141-93-5, 1,3-Diethylbenzene 150-78-7, 1,4-Dimethoxybenzene 198-55-0, Perylene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 218-01-9, Chrysene 301-02-0 496-11-7, 2,3-Dihydro-1H-indene 504-20-1 514-94-3, 1,5,5,6-Tetramethyl-1,3-cyclohexadiene 514-96-5, 1,2,6,6-Tetramethyl-1,3-cyclohexadiene 526-73-8, 1,2,3-Trimethylbenzene 535-77-3, 1-Methyl-3-(1-methylethyl)benzene 538-58-9, 1,5-Diphenyl-1,4-pentadien-3-one 546-49-6, 3,3,6-Trimethyl-1,5-heptadien-4-one 586-62-9 604-53-5, 1,1'-Binaphthalene 611-14-3, 1-Ethyl-2-methylbenzene 612-78-2, 2,2'-Binaphthalene 620-14-4, 1-Ethyl-3-methylbenzene 622-96-8, 1-Ethyl-4-methylbenzene 629-50-5, Tridecane 629-59-4, Tetradecane 1074-17-5, 1-Methyl-2-propylbenzene 1074-43-7, 1-Methyl-3-propylbenzene 1090-13-7, 5,12-Naphthacenedione 1120-21-4, Undecane 1193-18-6, 3-Methyl-2-cyclohexen-1-one 1515-95-3, 1-Ethyl-4-methoxy-benzene 2464-33-7 2819-61-6 3211-80-1 3212-51-9 3431-87-6 3561-67-9 3637-01-2, 1-(3,4-Dimethylphenyl)-ethanone 4325-74-0, 1,2'-Binaphthalene 17851-53-5, 1,2-Benzenedicarboxylic acid, butyl-2-methylpropyl ester 62968-85-8 66378-50-5, 2-Acetyl-2-carene 72535-88-7 74381-40-1, Propanoic acid, 2-methyl-,1(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester 77822-60-7 197390-29-7 208179-76-4
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

(org. pollutant detn. in contaminated soils)

REFERENCE 2

AN 125:41250 CA
TI Analysis of extractable organic compounds in water by gas chromatography mass spectrometry: applications to surface water
AU Deroux, J. M.; Gonzalez, C.; Le Cloirec, P.; Kovacsik, G.
CS Lab. Genie Environ. Ind., Ecole Mines Ales, Fr.
SO Talanta (1996), 43(3), 365-380
CODEN: TLNTA2; ISSN: 0039-9140
DT Journal
LA English
CC 61-3 (Water)
Section cross-reference(s): 80
AB Over a period of 1 yr, the surface water of a canal network (Languedoc-Roussillon area, France) was analyzed in order to identify org. compds. and to monitor its quality. Pollutants were extd. from 19 L of raw water using methylene chloride in a continuous countercurrent liq.-liq. extractor with a pulsed column. The extn. was performed at a pH above 11 and again at a pH below 2 according to U.S. Environmental Protection Agency method 625. The ext. was analyzed by gas chromatog./mass spectrometry, using two ionization techniques, namely electron ionization and chem. ionization. Mass spectra obtained by electron ionization were compared with those in a database (NIST). Some natural compds. and micropollutants were identified. Their structures were confirmed by chem. ionization (methane). One hundred and ten substances, making up the broad spectrum of extractable compds. in the surface water studied, were found by this method at a nanogram per L concn. level. Among them, 13 are priority pollutants. These specific pollutants were qualified.
ST extractable org detn surface water GCMS
IT Water pollution
(anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT Chlorides, analysis
RL: ANT (Analyte); ANST (Analytical study)
(anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT Pesticides
(detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)
IT Alcohols, analysis
Aldehydes, analysis
Amines, analysis
Aromatic hydrocarbons, analysis
Ketones, analysis
Phenols, analysis
RL: ANT (Analyte); ANST (Analytical study)
(detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)
IT Organic compounds, analysis
RL: ANT (Analyte); ANST (Analytical study)
(sulfur-contg., anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT 74-82-8, Methane, analysis 75-09-2, analysis 7440-61-1, Uranium, analysis 7704-34-9D, Sulfur, org. compds.
RL: ANT (Analyte); ANST (Analytical study)
(anal. of extractable org. compds. in water by gas chromatog. mass spectrometry: applications to surface water)
IT 62-53-3, Benzenamine, analysis
RL: ANT (Analyte); ANST (Analytical study)
(derivs; detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)

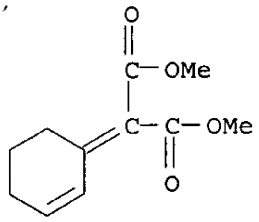
IT 7732-18-5, Water, analysis
RL: AMX (Analytical matrix); ANST (Analytical study)
(detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)

IT 51-28-5, analysis 58-08-2, analysis 58-89-9 65-85-0, Benzoic acid, analysis 78-40-0 80-46-6 83-32-9 83-33-0 86-73-7, 9H-Fluorene 87-28-5 87-41-2, 1(3H)-Isobenzofuranone 87-61-6 87-65-0 88-06-2 88-72-2 88-75-5 88-85-7 89-64-5 91-56-5, 1H-Indole-2,3-dione 91-64-5, 2H-1-Benzopyran-2-one 92-48-8, 6-Methyl-2H-1-benzopyran-2-one 95-65-8 95-76-1 98-54-4 98-73-7, p-tert-Butylbenzoic acid 98-95-3, analysis 99-30-9 99-52-5 99-54-7 99-96-7, analysis 99-99-0 100-00-5 100-18-5 100-46-9, Benzenemethanamine, analysis 101-84-8 103-69-5 115-96-8 120-12-7, Anthracene, analysis 121-14-2 122-34-9 122-95-2 127-51-5 130-15-4, 1,4-Naphthalenedione 132-64-9, Dibenzofuran 137-17-7 140-67-0 150-78-7 206-44-0, Fluoranthene 298-00-0 487-48-9 496-15-1 497-56-3, 2-Methyl-3,5-dinitrophenol 523-80-8 529-16-8, 2,3-Dimethyl-bicyclo[2,2,1]hept-2-ene 583-60-8 606-20-2 609-89-2 611-06-3 611-92-7 618-45-1, 3-(1-Methylethyl)phenol 619-08-9 620-02-0, 5-Methyl-2-furancarboxaldehyde 620-83-7, 1-Methyl-4-(phenylmethyl)benzene 634-93-5 696-23-1 700-38-9 759-22-8, N,N'-Bis(1-methylethyl)acetamide 816-16-0 825-41-2 873-94-9 931-54-4 1125-21-9 1195-79-5, 1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one 1635-02-5 1689-64-1, 9H-Fluoren-9-ol 1817-47-6, 1-(1-Methylethyl)-4-nitrobenzene 1912-24-9 1984-65-2 2189-60-8 2605-67-6, (Triphenylphosphoranylidene) methyl acetate 2683-43-4 3211-80-1 3302-10-1 3552-33-8 5590-14-7, 2-Phenyl-trans-cyclopropanecarbonitrile 5715-23-1 5915-41-3 6333-37-5 6341-97-5 6781-42-6 7051-39-0 7789-92-6 10298-80-3 13524-76-0, 3,3-Dimethyl-2(3H)-benzofuranone 13757-91-0 15176-21-3 15356-74-8 15972-60-8 17699-14-8, .alpha.-Cubebene 20547-99-3 20895-41-4, 6-Methyl-3(2H)-benzofuranone 21303-80-0, Dihydro-5-methyl-5-phenyl-2(3H)-furanone 22841-82-3 26271-75-0, 4-Amino-3,5-dichlorophenol 26545-51-7 51218-45-2 53543-47-8 54120-64-8 160498-63-5, 2,3-Dihydro-2,3-dimethyl-7-benzofuranol
RL: ANT (Analyte); ANST (Analytical study)
(detn. of extractable org. compds. in surface water by gas chromatog. mass spectrometry)

RN 122471-20-9 REGISTRY
CN Propanedioic acid, 2-cyclohexen-1-ylidene-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H14 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, GMELIN*
(*File contains numerically searchable property data)

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |



Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|---|---|---|
| Bioconc. Factor (BCF) | 33.9 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 33.9 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 33.9 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 33.9 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 33.9 | pH 10 | (1) ACD |
| Boiling Point (BP) | 258.1+/-13.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (HVAP) | 49.57+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 119.6+/-32.8 deg C | | (1) ACD |
| Freely Rotatable Bonds (FRB) | 4 | | (1) ACD |
| H acceptors (HAC) | 4 | | (1) ACD |
| H donors (HD) | 0 | | (1) ACD |
| Koc (KOC) | 433 | pH 1 | (1) ACD |
| Koc (KOC) | 433 | pH 4 | (1) ACD |
| Koc (KOC) | 433 | pH 7 | (1) ACD |
| Koc (KOC) | 433 | pH 8 | (1) ACD |
| Koc (KOC) | 433 | pH 10 | (1) ACD |
| logD (LOGD) | 2.32 | pH 1 | (1) ACD |
| logD (LOGD) | 2.32 | pH 4 | (1) ACD |
| logD (LOGD) | 2.32 | pH 7 | (1) ACD |
| logD (LOGD) | 2.32 | pH 8 | (1) ACD |
| logD (LOGD) | 2.32 | pH 10 | (1) ACD |
| logP (LOGP) | 2.316+/-0.350 | | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |

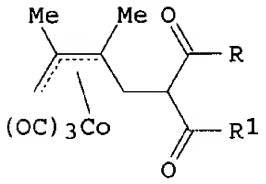
| | | | |
|---|---|---|---|
| Molecular Weight (MW) | 210.23 | | (1) ACD |
| Vapor Pressure (VP) | 0.0139633 Torr | 25.0 deg C | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

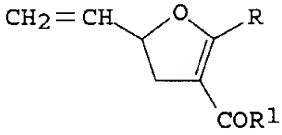
1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

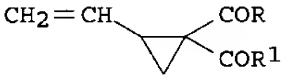
AN 111:154088 CA
TI Deprotonation of the adducts of .beta.-dicarbonyl anions and [(.eta.4-diene)Co(CO)3]BF4
AU Barinelli, Lucio S.; Li, Zhong; Nicholas, Kenneth M.
CS Dep. Chem. Biochem., Univ. Oklahoma, Norman, OK, 73019, USA
SO Organometallics (1989), 8(10), 2474-6
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 24, 27
GI




II




III




IV

AB The adducts of stabilized enolates and [(.eta.4-1,3-butadiene)Co(CO)3]BF4 (I) and [(.eta.4-1,3-cyclohexadiene)Co(CO)3]BF4 undergo deprotonation and subsequent reactions to form either hydrofurans, cyclopropanes, or .alpha.,.beta.,.gamma.,.delta.-diunsatd. dicarbonyl derivs. depending upon the reacting complex and the .beta.-dicarbonyl component. All of the obsd. reactions are strongly promoted by HMPA. Thus, treatment of the adducts II (R = Me, R1 = Ph, OMe; R = R1 = OMe), formed from reaction of I and RCOCH:C(ONa)R1, with LiN(CHMe2)2 in the presence of HMPA give dihydrofurans III (R = Me, R1 = Ph, OMe) or cyclopropane IV (R = R1 = OMe).

ST enolate dienecobalt alkylation; deprotonation dienecobalt enolate adduct cyclization; HMPA deprotonation catalyst dienecobalt enolate adduct; hydride shift dienecobalt enolate adduct; dihydrofuran vinyl acyl; cyclopropane vinyl diacyl

IT Ring closure and formation
(in deprotonation of adducts of stabilized enolates with (diene)cobalt tricarbonyl cations)

IT Hydride shift
(1,4-, in deprotonation reactions of adducts of .beta.-dicarbonyl anions with (diene)cobalt tricarbonyl cations)

IT Protonation catalysts
(deprotonation, HMPA, for adducts of .beta.-dicarbonyl anions and (diene)cobalt tricarbonyl cations)

IT Protonation and Proton transfer reaction
(deprotonation, of adducts of .beta.-dicarbonyl anions and (diene)cobalt tricarbonyl cations)

IT 623-58-5, Sodium acetoacetate 17664-05-0, Sodium benzoylacetonate 18424-76-5, Sodium dimethyl malonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of enolate adducts of (diene)cobalt tricarbonyl cations)

IT 680-31-9, HMPA, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalyst, in deprotonation of enolate adducts of (diene)cobalt tricarbonyl cation)

IT 33009-59-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage of, (dimethylbutadiene)cobalt tricarbonyl cation from)

IT 1333-74-0 12184-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride shift, 1,4-, in deprotonation reactions of adducts of .beta.-dicarbonyl anions with (diene)cobalt tricarbonyl cations)

IT 122471-24-3P 122471-25-4P 122471-27-6P 122471-28-7P 122471-29-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deprotonation of)

IT 122471-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and C-alkylation of, with stabilized enolates)

IT 17447-60-8P 34939-28-1P 88326-56-1P 113949-31-8P 115740-69-7P 122471-14-1P 122471-15-2P 122471-16-3P 122471-17-4P 122471-18-5P 122471-19-6P 122471-20-9P 122471-26-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 122471-23-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., hydrolysis, and deprotonation of)

IT 12408-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation and Proton transfer reaction, deprotonation, of adducts of .beta.-dicarbonyl anions and (diene)cobalt tricarbonyl cations)

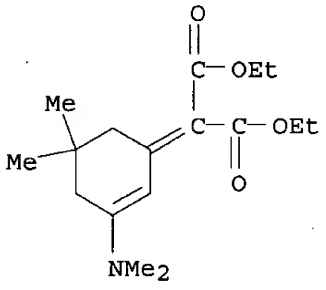
IT 90502-48-0 113949-35-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(C-alkylation of, with stabilized enolates)

RN 31039-90-4 REGISTRY
CN 2-Cyclohexene-.DELTA.1,.alpha.-malonic acid, 3-(dimethylamino)-5,5-dimethyl-, diethyl ester (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H27 N O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |

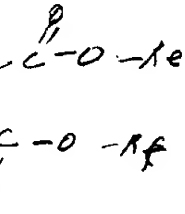
cl 1




1
4
7

D = $NR_aR_b$ $R_a = R_b = Me$

$R_e, R_f = CH_3$

A = 

$R_c = R_f = Et$

Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|---|---|---|
| Bioconc. Factor (BCF) | 1 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 1.57 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 435 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 774 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 846 | pH 10 | (1) ACD |
| Boiling Point (BP) | 359.3+/-42.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (HVAP) | 60.48+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 171.1+/-50.2 deg C | | (1) ACD |
| Freely Rotatable Bonds (FRB) | 7 | | (1) ACD |
| H acceptors (HAC) | 5 | | (1) ACD |
| H donors (HD) | 0 | | (1) ACD |
| Koc (KOC) | 3.45 | pH 1 | (1) ACD |
| Koc (KOC) | 8.01 | pH 4 | (1) ACD |
| Koc (KOC) | 2226 | pH 7 | (1) ACD |
| Koc (KOC) | 3961 | pH 8 | (1) ACD |
| Koc (KOC) | 4332 | pH 10 | (1) ACD |
| logD (LOGD) | 1.06 | pH 1 | (1) ACD |
| logD (LOGD) | 1.42 | pH 4 | (1) ACD |
| logD (LOGD) | 3.87 | pH 7 | (1) ACD |
| logD (LOGD) | 4.12 | pH 8 | (1) ACD |
| logD (LOGD) | 4.15 | pH 10 | (1) ACD |
| logP (LOGP) | 4.156+/-0.387 | | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD |

| | | | |
|---|---|---|---|
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |
| Molecular Weight (MW) | 309.40 | | (1) ACD |
| pKa (PKA) | 6.98+/-0.20 | Most Basic | (1) ACD |
| Vapor Pressure (VP) | 2.41E-05 Torr | 25.0 deg C | (1) ACD |

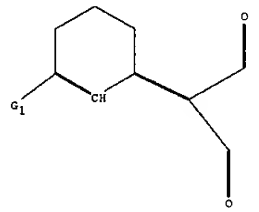
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

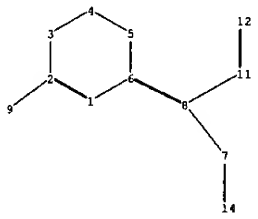
1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 74:12468 CA
TI Hindered internal rotation in some enamines
AU Dahlqvist, Kjell I.; Forsen, Sture
CS Chem. Cent., Lund Inst. Technol., Lund, Swed.
SO Acta Chemica Scandinavica (1947-1973) (1970), 24(6), 2075-83
CODEN: ACSAA4; ISSN: 0001-5393
DT Journal
LA English
CC 22 (Physical Organic Chemistry)
GI For diagram(s), see printed CA Issue.
AB The hindered internal rotation of the N,N-dimethyl group in I, II, and III was studied by NMR at 60 and 100 MHz. The interconversion rate was evaluated by iterative fitting of the theoretical spectra to the exptl. spectra using digital computer. The free energy of activation (.DELTA.F.++.) for the hindered internal rotation of NMe in the compds. studied depends on the exocyclic substituent in the order :C(COOEt)2 <:O <:C(CN)2. The entropies of activation had large pos. values.
ST cyclohexene enamines hindered internal rotation; enamines cyclohexene hindered internal rotation; hindered internal rotation cyclohexene enamines
IT Amines, properties
RL: PRP (Properties)
(enamines, potential barrier to rotation of)
IT Entropy
Free energy
(of activation, of rotation of enamines)
IT Potential barriers
(rotational, of enamines)
IT 31039-88-0 31039-89-1 31039-90-4
RL: PRP (Properties)
(potential barrier to rotation of)
IT 31039-91-5P 31039-92-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

C:\STNEXP4\QUERIES\285937a.str




chain nodes :
7 8 9 11 12 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-9 6-8 7-8 7-14 8-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-9 3-4 4-5 5-6 7-14 11-12
exact bonds :
6-8 7-8 8-11

G1:C,H,O,S,N,P

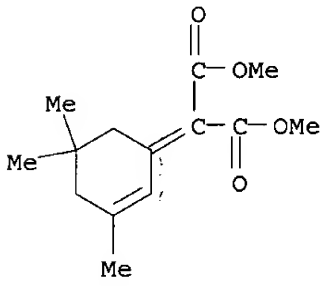
G2:C,H,O,N,p-C6H4,CO2H,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 14:CLASS

RN 124648-10-8 REGISTRY
CN Propanedioic acid, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H20 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |



A : $COOR_e$ $R_e, R_f = Me$
$COOR_f$

(D $= CH_3$, $R_o, R_p = CH_3$

Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|---|---|---|
| Bioconc. Factor (BCF) | 580 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 580 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 580 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 580 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 580 | pH 10 | (1) ACD |
| Boiling Point (BP) | 291.1+/-13.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (HVAP) | 53.05+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 132.2+/-32.8 deg C | | (1) ACD |
| H acceptors (HAC) | 4 | | (1) ACD |
| H donors (HD) | 0 | | (1) ACD |
| Koc (KOC) | 3309 | pH 1 | (1) ACD |
| Koc (KOC) | 3309 | pH 4 | (1) ACD |
| Koc (KOC) | 3309 | pH 7 | (1) ACD |
| Koc (KOC) | 3309 | pH 8 | (1) ACD |
| Koc (KOC) | 3309 | pH 10 | (1) ACD |
| logD (LOGD) | 3.94 | pH 1 | (1) ACD |
| logD (LOGD) | 3.94 | pH 4 | (1) ACD |
| logD (LOGD) | 3.94 | pH 7 | (1) ACD |
| logD (LOGD) | 3.94 | pH 8 | (1) ACD |
| logD (LOGD) | 3.94 | pH 10 | (1) ACD |
| logP (LOGP) | 3.939+/-0.367 | | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |

| | | | |
|---|---|---|---|
| Molecular Weight (MW) | 252.31 | | (1) ACD |
| Vapor Pressure (VP) | 0.00199311 Torr | 25.0 deg C | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

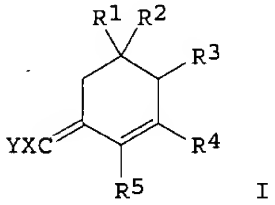
1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 112:42246 CA
TI Cyclohexenylidenes as sunscreen agents
IN Cleary, Thomas P.; Gosciniak, Donald J.; Phalangas, Charalambos J.
PA ICI Americas, Inc., USA
SO U.S., 7 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K007-40
ICS A61K007-42; A61K007-44; A61K009-10
NCL 424059000
CC 62-4 (Essential Oils and Cosmetics)
Section cross-reference(s): 24
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 4847073 | A | 19890711 | US 1988-212824 | 19880629 |
| | BR 8903225 | A | 19910102 | BR 1989-3225 | 19880629 |
| | EP 349139 | A2 | 19900103 | EP 1989-305854 | 19890609 |
| | EP 349139 | A3 | 19900530 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | ZA 8904488 | A | 19900725 | ZA 1989-4488 | 19890613 |
| | AU 8936362 | A1 | 19900104 | AU 1989-36362 | 19890614 |
| | AU 616273 | B2 | 19911024 | | |
| | FI 8903132 | A | 19891230 | FI 1989-3132 | 19890627 |
| | JP 02153988 | A2 | 19900613 | JP 1989-168256 | 19890629 |
| PRAI | US 1988-212824 | 19880629 | | | |
| | GB 1989-13345 | 19890609 | | | |

GI




I

AB Sunscreen compns. contain cyclohexenylidenes (I: X, Y = CN, CO2R6, CONHR6, CONR32, PhCO2R6, PhCOR6, PhNR32, only one X or Y may be substituted with H; R1-R5 = H, OH, CO2R6, alkyl, alkoxy, hydroxyalkyl; R6 = H, alkyl, alkylaryl, arylalkyl) as UV filters. I provide selected absorption of actinic radiation in the UV-B as well as UV-A range. A mixt. contg. I (R1-R3 = H, R4 = Me, R5 = H, X = CN, Y = CO2Me)(II) 8% and dimethylisosorbide 92% was applied to excised hairless mouse epidermis at 1 mg/cm2 and the epidermis was exposed to UV radiation and the skin protection factor was measured to be 14.0 in the UV-B range and 1.73 in the UV-A range. A sunscreen lotion contained II 5.00, petrolatum 35.00, Brij-721 1.16, Brij-72 3.86, silicone oil 3.00, Uvinul M-40 3.00, water 48.08, Carbopol-934 0.40, NaOH (10% aq. soln.) 0.40, and Dowicil-200

0.10%.

ST sunscreen cyclohexenylidene cyanoacetate prepn

IT Polishing materials
(cyclohexenylidenes in, as sunscreen agents)

IT Hair preparations
Sunburn and Suntan
(sunscreens, cyclohexenylidenes in)

IT 109-73-9, Butylamine, biological studies
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of cyclohexenylidene cyanoacetic acid chloride)

IT 78-59-1, Isophorone
RL: BIOL (Biological study)
(condensation of, with Me cyanoacetate)

IT 62-53-3, Aniline, biological studies 67-63-0, Isopropanol, biological studies 126-30-7, 2,2-Dimethyl-1,3-propanediol
RL: BIOL (Biological study)
(condensation of, with cyclohexenylidene cyanoacetate)

IT 105-34-0, Methyl cyanoacetate 108-59-8, Dimethyl malonate
RL: BIOL (Biological study)
(condensation of, with isophorone)

IT 124648-13-1P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and amidation of, with butylamine)

IT 56058-30-1P 124648-14-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with Et cyanoacetate)

IT 80699-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with crotonaldehyde)

IT 30525-89-4, Paraformaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et acetoacetate)

IT 4170-30-3, Crotonaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isophorone silyl enol ether)

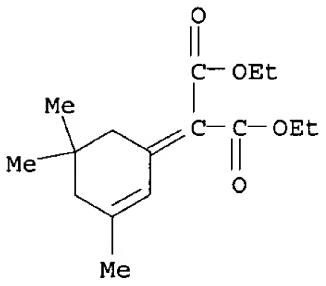
IT 141-97-9, Ethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with paraformaldehyde)

IT 20159-49-3 23051-44-7 52903-68-1 52903-69-2 55952-69-7
88973-42-6 107100-75-4 124647-97-8 124647-98-9 124647-99-0
124648-00-6 124648-01-7 124648-02-8 124648-03-9 124648-04-0
124648-05-1 124648-06-2 124648-07-3 124648-08-4 124648-09-5
124648-10-8 124648-11-9 124648-12-0
RL: BIOL (Biological study)
(sunscreen agent)

RN 41589-44-0 REGISTRY
CN Propanedioic acid, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H24 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |




Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|---|---|---|
| Bioconc. Factor (BCF) | 3725 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 3725 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 3725 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 3725 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 3725 | pH 10 | (1) ACD |
| Boiling Point (BP) | 325.0+/-15.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (HVAP) | 56.71+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 148.6+/-33.8 deg C | | (1) ACD |
| Freely Rotatable Bonds (FRB) | 6 | | (1) ACD |
| H acceptors (HAC) | 4 | | (1) ACD |
| H donors (HD) | 0 | | (1) ACD |
| Koc (KOC) | 12526 | pH 1 | (1) ACD |
| Koc (KOC) | 12526 | pH 4 | (1) ACD |
| Koc (KOC) | 12526 | pH 7 | (1) ACD |
| Koc (KOC) | 12526 | pH 8 | (1) ACD |
| Koc (KOC) | 12526 | pH 10 | (1) ACD |
| logD (LOGD) | 5.00 | pH 1 | (1) ACD |
| logD (LOGD) | 5.00 | pH 4 | (1) ACD |
| logD (LOGD) | 5.00 | pH 7 | (1) ACD |
| logD (LOGD) | 5.00 | pH 8 | (1) ACD |
| logD (LOGD) | 5.00 | pH 10 | (1) ACD |
| logP (LOGP) | 5.002+/-0.367 | | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD |

| | | | |
|---|---|---|---|
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |
| Molecular Weight (MW) | 280.36 | | (1) ACD |
| Vapor Pressure (VP) | 0.000236805 Torr | 25.0 deg C | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

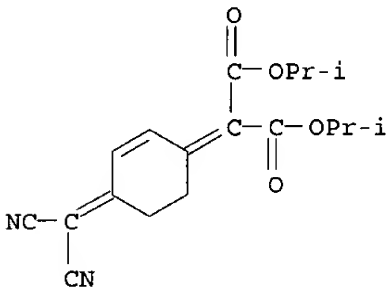
REFERENCE 1

AN 78:158864 CA
TI Knoevenagel condensations with titanium tetrachloride-base. III. Reaction of ketones and .alpha.-halo ketones with malonate
AU Lehnert, W.
CS Univ.-Kinderklin., Freiburg, Fed. Rep. Ger.
SO Tetrahedron (1973), 29(4), 635-8
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA German
CC 23-16 (Aliphatic Compounds)
Section cross-reference(s): 24, 25, 26
AB Condensation of H2C(CO2Et)2 with aliph., arom., and cyclic ketones, RR1CO, in the presence of TiCl4-pyridine gave 42-96% RR1C:C(CO2Et)2..alpha.-Mono-,.alpha.,.alpha.-di-, and .alpha.,.alpha.,.alpha.-trihalo ketones reacted similarly.
ST Knoevenagel malonate ketone; halo ketone malonate Knoevenagel; titanium chloride Knoevenagel
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel condensation of, with diethyl malonate)
IT Knoevenagel reaction
(of ketones with diethyl malonate in presence of titanium tetrachloride-pyridine)
IT 7550-45-0, uses and miscellaneous
RL: USES (Uses)
(Knoevenagel condensation of ketones with diethyl malonate in presence of pyridine and)
IT 110-86-1, uses and miscellaneous
RL: USES (Uses)
(Knoevenagel condensation of ketones with diethyl malonate in presence of titanium tetrachloride and)
IT 108-59-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel condensation of, with bicycloheptanone)
IT 67-64-1, reactions 78-59-1 78-93-3, reactions 78-95-5 108-94-1, reactions 119-61-9, reactions 120-92-3 123-19-3 134-81-6 421-50-1 486-25-9 497-38-1 532-27-4 534-07-6 1191-95-3 2648-61-5 4091-39-8 6317-49-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel condensation of, with diethyl malonate)
IT 105-53-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Knoevenagel condensation with ketones of, in presence of titanium tetrachloride-pyridine)
IT 6802-75-1P 24824-36-0P 41589-39-3P 41589-40-6P 41589-41-7P 41589-42-8P 41589-43-9P 41589-44-0P 41589-45-1P 41589-46-2P 41589-48-4P 41589-49-5P 41589-50-8P 41589-51-9P 41589-52-0P 41589-53-1P 41589-54-2P 41649-47-2P 41649-48-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 199384-77-5 REGISTRY
CN Propanedioic acid, [4-(dicyanomethylene)-2-cyclohexen-1-ylidene]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H20 N2 O4
SR CA
LC STN Files: CA, CAPLUS

Ring System Data

| Elemental Analysis EA | Elemental Sequence ES | Size of the Rings SZ | Ring System Formula RF | Ring Identifier RID | RID Occurrence Count |
|---|---|---|---|---|---|
| C6 | C6 | 6 | C6 | 46.150.2 | 1 |




Calculated Properties (CALC)

| PROPERTY (CODE) | VALUE | CONDITION | NOTE |
|---|---|---|---|
| Bioconc. Factor (BCF) | 98.8 | pH 1 | (1) ACD |
| Bioconc. Factor (BCF) | 98.8 | pH 4 | (1) ACD |
| Bioconc. Factor (BCF) | 98.8 | pH 7 | (1) ACD |
| Bioconc. Factor (BCF) | 98.8 | pH 8 | (1) ACD |
| Bioconc. Factor (BCF) | 98.8 | pH 10 | (1) ACD |
| Boiling Point (BP) | 421.9+/-45.0 deg C | 760.0 Torr | (1) ACD |
| Enthalpy of Vap. (HVAP) | 67.60+/-3.0 kJ/mol | | (1) ACD |
| Flash Point (FP) | 184.4+/-34.1 deg C | | (1) ACD |
| Freely Rotatable Bonds (FRB) | 6 | | (1) ACD |
| H acceptors (HAC) | 6 | | (1) ACD |
| H donors (HD) | 0 | | (1) ACD |
| Koc (KOC) | 932 | pH 1 | (1) ACD |
| Koc (KOC) | 932 | pH 4 | (1) ACD |
| Koc (KOC) | 932 | pH 7 | (1) ACD |
| Koc (KOC) | 932 | pH 8 | (1) ACD |
| Koc (KOC) | 932 | pH 10 | (1) ACD |
| logD (LOGD) | 2.93 | pH 1 | (1) ACD |
| logD (LOGD) | 2.93 | pH 4 | (1) ACD |
| logD (LOGD) | 2.93 | pH 7 | (1) ACD |
| logD (LOGD) | 2.93 | pH 8 | (1) ACD |
| logD (LOGD) | 2.93 | pH 10 | (1) ACD |
| logP (LOGP) | 2.928+/-0.437 | | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 1 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 4 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 7 | (1) ACD |
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 8 | (1) ACD |

| | | | |
|---|---|---|---|
| Molar Solubility (SLB.MOL) | <0.01 mol/L | pH 10 | (1) ACD |
| Molecular Weight (MW) | 328.36 | | (1) ACD |
| Vapor Pressure (VP) | 2.51E-07 Torr | 25.0 deg C | (1) ACD |

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 128:23197 CA
TI Synthesis and polymerization of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes
AU Itoh, Takahito; Okuno, Hiroyuji; Hishida, Takeshi; Inokuchi, Akira; Kamei, Nobuaki; Sato, Tamotsu; Kubo, Masataka; Iwatsuki, Shouji
CS Dep. Chem. Mater., Fac. Eng., Mie Univ., Mie, 514, Japan
SO Tetrahedron (1997), 53(45), 15247-15261
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English
CC 35-4 (Chemistry of Synthetic High Polymers)
AB Attempts were made to prep. novel 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes [ethoxy(5a), isopropoxy(5b), and tert-butoxy(5c)], 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes [ethoxy(6a), isopropoxy(6b), and tert-butoxy(6c)], and 1-(2,2-dimethyl-1,3-dioxane-4,6-dione-5-ylidene)-4-(dicyanomethylene)-2,5-cyclohexadiene(6d). 5C and 6d were obtained as yellow and orange needles, resp., but 5a, 5b and 6a-c could not be isolated as crystals. Homopolymns. of 5c and 6d and their copolymns. with styrene were studied.
ST alkoxycarbonyltricyanoquinodimethane bisalkoxycarbonyldicyanoquinodimethane prepn polymn
IT Polymerization
Polymerization catalysts
(ionic; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
IT Polymerization
Polymerization catalysts
(radical; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
IT Cardo polymers
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and polymn. of 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
IT Solvent effect
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
IT 199384-59-3P 199384-60-6P 199384-61-7P 199384-62-8P 199384-63-9P 199384-64-0P 199384-65-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)
IT 78-67-1, AIBN 109-63-7, Boron trifluoride etherate 109-72-8, Butyl lithium, uses 121-44-8, uses 616-45-5, Pyrrolidone
RL: CAT (Catalyst use); USES (Uses)
(polymn. catalyst; synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-

tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-69-5P 199384-70-8P 199384-71-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 105-53-3, Diethyl malonate 109-77-3, Malonodinitrile 541-16-2, Di(tert-butyl) malonate 2033-24-1, Isopropylidene malonate 13195-64-7, Diisopropyl malonate 83928-81-8 83928-82-9 145984-88-9 156879-16-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-66-2P 199384-67-3P 199384-68-4P 199384-72-0P 199384-73-1P 199384-74-2P 199384-75-3P 199384-76-4P 199384-77-5P 199384-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

IT 199384-79-7P 199384-80-0P 199384-81-1P 199384-82-2P 199384-83-3P 199384-84-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and polymn. of 7-alkoxycarbonyl-7,8,8-tricyanoquinodimethanes and 7,7-bis(alkoxycarbonyl)-8,8-dicyanoquinodimethanes)

AN 2000:409546 CAPLUS
DN 133:230235
TI Influence of the chromophore ionization potential on speed and magnitude of photorefractive effects in poly(N-vinylcarbazole) based polymer composites
AU Van Steenwinckel, David; Hendrickx, Eric; Persoons, Andre; Van den Broeck, Kurt; Samyn, Celest
CS Center for Research on Molecular Electronics and Photonics, Laboratory for Chemical and Biological Dynamics, University of Leuven, Louvain, B-3001, Belg.
SO J. Chem. Phys. (2000), 112(24), 11030-11037
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 73
AB The authors report on the synthesis of three highly polar chromophores and their use as **dopants** in poly(N-vinylcarbazole) based photorefractive polymer composites sensitized with (2,4,7-trinitro-9-fluorenylidene)malononitrile. Small alterations in the amino donor group substituents were used to tune the dye's ionization potential (IP) by 0.2 eV. At 780 nm, 5 .degree.C above the glass transition temp. (Tg), and with an applied field of 59 V/.mu.m, the authors obsd. complete internal diffraction and a gain coeff. of 167 cm-1. In this temp. range, diffraction efficiency, gain coeff., and photorefractive phase shift were found to correlate with the chromophore IP. At 20 .degree.C Tg, the contribution from birefringence to the index modulation was insignificant, and the speed of the photorefractive effect correlated well with the chromophore IP. Anal. of the results suggests that the space-charge field was influenced by the chromophore IP.
ST photorefractive effect polyvinylcarbazole based polymer composite; chromophore ionization potential photorefractive effect polyvinylcarbazole based polymer composite
IT Ionization potential
Photorefractive effect
Photorefractive gratings
(chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)
IT **149227-09-8 190715-16-3 190715-17-4**
RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
(chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)
IT 25067-59-8, Poly(N-vinylcarbazole)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(chromophore **dopant** ionization potential effect on

photorefractive effects in poly(vinylcarbazole) based polymer composites)

IT 86-28-2, N-Ethylcarbazole
RL: NUU (Nonbiological use, unclassified); USES (Uses)
(plasticizer; chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)

IT 1201-91-8, 4-[N-(2-Hydroxyethyl)-N-methylamino]benzaldehyde 4181-05-9, p-N,N-Diphenylaminobenzaldehyde 42906-19-4, 4-N,N-Di-(p-tolyl)aminobenzaldehyde
RL: RCT (Reactant)
(reaction with (trimethylhexeneylidene)propanedinitrile)

IT **23051-44-7**
RL: RCT (Reactant)
(reaction with aminobenzaldehydes)

IT 1172-02-7, 2,4,7-Trinitro-9-fluorenylidene)malononitrile
RL: MOA (Modifier or additive use); USES (Uses)
(sensitizer; chromophore **dopant** ionization potential effect on photorefractive effects in poly(vinylcarbazole) based polymer composites)

RE.CNT 29

RE

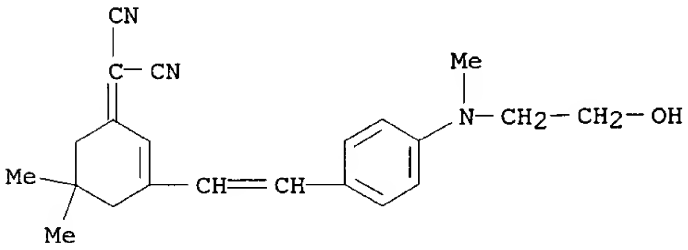

(1) Ambrose, J; J Electrochem Soc 1968, V115, P1159 CAPLUS
(2) Bassler, H; Phys Status Solidi B 1993, V175, P15
(3) Ducharme, S; Phys Rev Lett 1991, V66, P1846 CAPLUS
(4) Elias, H; Macromolecules 1983, P375
(5) Golemme, A; Opt Lett 1997, V22, P1226 CAPLUS
(6) Grunnet-Jepsen, A; Chem Phys Lett 1998, V291, P553 CAPLUS
(7) Gunter, P; Photorefractive Materials and Their Applications 1988, V1-2
(8) Hendrickx, E; Appl Phys Lett 1997, V71, P1159 CAPLUS
(9) Hendrickx, E; Chem Phys 1999, V245, P407 CAPLUS
(10) Herlocker, J; Appl Phys Lett 1999, V74, P2253 CAPLUS
(11) Khoo, C; Opt Lett 1994, V19, P1723
(12) Kippelen, B; J Am Chem Soc 1997, V119, P4559 CAPLUS
(13) Kippelen, B; Nonlinear Optics of Organic Molecules and Polymers 1997, P465
CAPLUS
(14) Kippelen, B; Science 1998, V279, P54 CAPLUS
(15) Kogelnik, H; Bell Syst Tech J 1969, V48, P2909
(16) Kukhtarev, N; Ferroelectrics 1979, V22, P949 CAPLUS
(17) Lemke, R; Synthesis 1974, V1, P359
(18) Lundquist, P; Science 1996, V274, P1182 CAPLUS
(19) Meerholz, K; Appl Phys Lett 1998, V73, P4 CAPLUS
(20) Meerholz, K; Nature 1994, V371, P497 CAPLUS
(21) Moerner, W; Annu Rev Mater Sci 1997, V27, P585 CAPLUS
(22) Moerner, W; J Chem Phys 1996, V105, P10637
(23) Pai, D; J Phys Chem 1984, V88, P4714 CAPLUS
(24) Reiss, H; J Phys Chem 1985, V89, P4207 CAPLUS
(25) Sandalphon, B; Appl Opt 1996, V35, P2346 CAPLUS
(26) Volodin, B; Opt Eng 1995, V34, P2213 CAPLUS
(27) Wu, J; J Opt Soc Am B 1991, V8, P142 CAPLUS
(28) Wurthner, F; Angew Chem Int Ed Engl 1997, V36, P2765 CAPLUS
(29) 's Heeren, G; Makromol Chem 1993, V194, P1773


IT **149227-09-8 190715-16-3 190715-17-4**
RL: MOA (Modifier or additive use); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process); USES (Uses)
(chromophore **dopant** ionization potential effect on

photorefractive effects in poly(vinylcarbazole) based polymer composites)

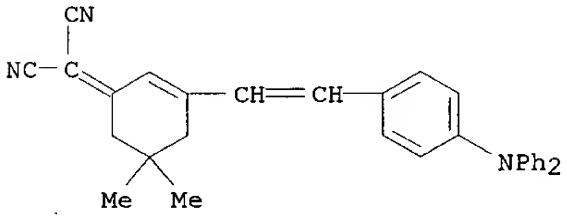
RN 149227-09-8 CAPLUS

CN Propanedinitrile, [3-[2-[4-[(2-hydroxyethyl)methylamino]phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



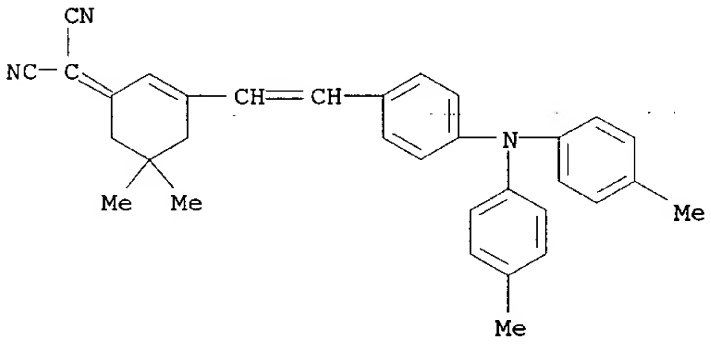
RN 190715-16-3 CAPLUS

CN Propanedinitrile, [3-[2-[4-(diphenylamino)phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



RN 190715-17-4 CAPLUS

CN Propanedinitrile, [3-[2-[4-[bis(4-methylphenyl)amino]phenyl]ethenyl]-5,5-dimethyl-2-cyclohexen-1-ylidene]- (9CI) (CA INDEX NAME)



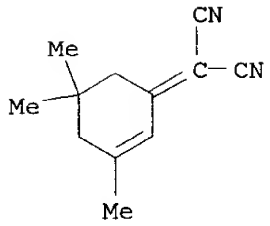
IT **23051-44-7**

RL: RCT (Reactant)

(reaction with aminobenzaldehydes)

RN 23051-44-7 CAPLUS

CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)

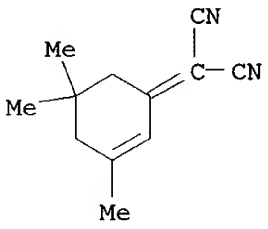

CN
Me
C— CN
Me
Me

AN 1999:601885 CAPLUS
DN 131:345185
TI Colorless high dielectric compounds for low voltage **liquid crystal** application
AU Wu, Shin-Tson; Schwartz, Robert N.; Zhang, Qing T.; Marder, Seth; Hsu, Chain-Shu
CS HRL Laboratories, Malibu, CA, 90265, USA
SO Mater. Res. Soc. Symp. Proc. (1999), 559(Liquid Crystal Materials and Devices), 235-242
CODEN: MRSPDH; ISSN: 0272-9172
PB Materials Research Society
DT Journal
LA English
CC 76-9 (Electric Phenomena)
Section cross-reference(s): 74, 75
AB Several colorless compds. with dielec. anisotropy in the 10-50 range were studied. The absorption spectra, phase transition temp., birefringence, dielec. anisotropy and viscoelastic coeff. of these compds. were measured.
ST dielec compd **liq crystal**
IT **Liquid crystal** displays
(active matrix; colorless high dielec. compds. for low voltage **liq. crystal** application)
IT Absorption spectra
Birefringence
Dielectric anisotropy
Dielectric constant
Electric insulators
**Liquid crystals**
Viscosity
(colorless high dielec. compds. for low voltage **liq. crystal** application)
IT Polyenes
RL: PRP (Properties)
(cyano-; colorless high dielec. compds. for low voltage **liq. crystal** application)
IT **23051-44-7** 27104-69-4 **30481-43-7** 68162-22-1
74240-64-5 74701-06-7 86776-50-3 117530-21-9 154195-65-0
190602-28-9 190602-29-0 190602-31-4 220036-97-5 **249934-22-3**
**249934-23-4** 249934-24-5
RL: PRP (Properties)
(colorless high dielec. compds. for low voltage **liq. crystal** application)
RE.CNT 18
RE
(1) Bahadur, B; Liquid Crystals: Applications and Uses 1992, V3
(2) Grant, B; Mol Cryst Liq Cryst 1978, V48, P175 CAPLUS
(3) Gray, G; Electron Lett 1973, V9, P130 CAPLUS
(4) Khoo, I; Optics and Nonlinear Optics of Liquid Crystals 1993
(5) Kippelen, B; Science 1998, V279, P54 CAPLUS
(6) Maier, W; Z Naturforsh Teil A 1960, V15, P287
(7) Sutherland, R; Proc SPIE 1998, V3421, P8 CAPLUS
(8) Szabo, A; Modern Quantum Chemistry 1989
(9) Tarao, R; SID Tech Digest 1994, V25, P233
(10) Wu, S; Appl Phys Lett 1992, V61, P630 CAPLUS
(11) Wu, S; Appl Phys Lett 1994, V64, P2191 CAPLUS
(12) Wu, S; Appl Phys Lett 1999, V74, P344 CAPLUS
(13) Wu, S; Asia Display'95 1995, P567

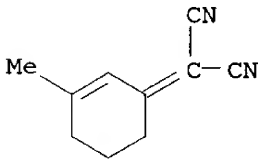
(14) Wu, S; Jpn J Appl Phys 1998, V37, PL1254 CAPLUS
(15) Wu, S; Jpn J Appl Phys 1999, V38, PL286 CAPLUS
(16) Wu, S; Opt Eng 1993, V32, P1792 CAPLUS
(17) Wu, S; Proc SPIE 1997, V3015, P8 CAPLUS
(18) Yang, D; Appl Phys Lett 1994, V64, P1905 CAPLUS

IT **23051-44-7 30481-43-7 249934-22-3**
**249934-23-4**
RL: PRP (Properties)
(colorless high dielec. compds. for low voltage **liq. crystal** application)

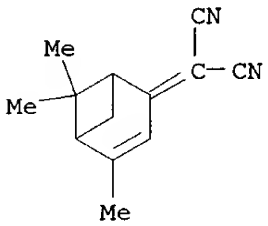
RN 23051-44-7 CAPLUS
CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)



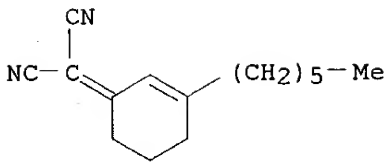

RN 30481-43-7 CAPLUS
CN Propanedinitrile, (3-methyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)




RN 249934-22-3 CAPLUS
CN Propanedinitrile, (4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-ylidene)- (9CI) (CA INDEX NAME)




RN 249934-23-4 CAPLUS
CN Propanedinitrile, (3-hexyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)


CN
NC
C
(CH2)5—Me

AN 2000:725601 CAPLUS
DN 133:303666
TI **Dopants** for **liquid crystal** devices
IN Wu, Shin-tson; Marder, Seth; Zhang, Qing T.
PA Hrl Laboratories, Llc, USA; California Institute of Technology
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C255-31
ICS C09K019-58
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 24, 75
FAN.CNT 1

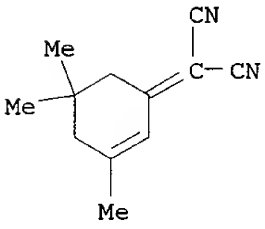
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2000059872 | A1 | 20001012 | WO 2000-US8488 | 20000329 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

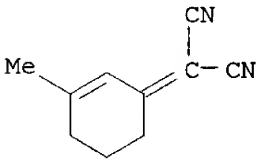
PRAI US 1999-285937 A1 19990402
AB High-dielec. colorless or virtually colorless **dopants** for low-voltage and tunable clearing temp. **liq. crystal** devices. These **dopant** compds. help reduce the operation voltage for both polar and non-polar **liq. crystal** (LC) mixts. Methods for making and using these **dopant** compds. are also disclosed.
ST **liq crystal** display **dopant**
IT **Dopants**
**Liquid crystal** displays
(**dopants** for **liq. crystal** devices)
IT **23051-44-7P 30481-43-7P 249934-23-4P 300859-99-8P**
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(**dopants** for **liq. crystal** devices)
IT 78-59-1 109-77-3, Malononitrile 1193-18-6 1196-01-6 3761-92-0, Hexylmagnesium bromide 5323-87-5 66262-12-2
RL: RCT (Reactant)
(**dopants** for **liq. crystal** devices)
RE.CNT 8
RE
(1) Anon; PATENT ABSTRACTS OF JAPAN 1985, V009(200), PC-298
(2) Gray, G; US 5456859 A 1995 CAPLUS
(3) Gudriniece, E; 1973, 9, P471 CAPLUS
(4) Gudriniece, E; LATV PSR ZINAT AKAD VESTIS, KIM SER 1972, V6, P722
(5) Hoechst Celanese Corp; EP 0530784 A 1993 CAPLUS
(6) Kantou Kagaku Kk; JP 60069059 A 1985 CAPLUS
(7) Kippelen, B; SCIENCE 1998, V279, P54 CAPLUS
(8) Leslie, G; US 2882158 A 1959 CAPLUS
IT **23051-44-7P 30481-43-7P 249934-23-4P**

**300859-99-8P**
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(**dopants** for **liq. crystal** devices)

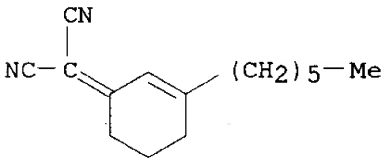
RN 23051-44-7 CAPLUS
CN Propanedinitrile, (3,5,5-trimethyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)




RN 30481-43-7 CAPLUS
CN Propanedinitrile, (3-methyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)

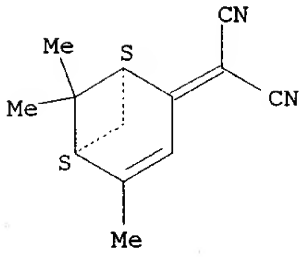



RN 249934-23-4 CAPLUS
CN Propanedinitrile, (3-hexyl-2-cyclohexen-1-ylidene)- (9CI) (CA INDEX NAME)




RN 300859-99-8 CAPLUS
CN Propanedinitrile, [(1S,5S)-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-ylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).


CN
Me
S
CN
Me
S
Me

AN 1992:407540 CAPLUS
DN 117:7540
ED Entered STN: 11 Jul 1992
TI Reactions of trifluoromethyl ketones. VIII. Investigation of steric effect of a trifluoromethyl group through ene reaction of trifluoromethyl ketones
AU Nagai, Takabumi; Nishioka, Goro; Koyama, Mayumi; Ando, Akira; Miki, Takuichi; Kumadaki, Itsumaro
CS Fac. Pharm. Sci., Setsunan Univ., Hirakata, 573-01, Japan
SO Chemical & Pharmaceutical Bulletin (1992), 40(3), 593-8
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 22
OS CASREACT 117:7540
AB In the ene reaction of trifluoromethyl ketones, a trifluoromethyl group has been obsd. to behave as a larger substituent than commonly believed in the biomedicinal field. To est. the steric effect of a trifluoromethyl group, several trifluoromethyl ketones RCOCF3 (R = H, Me, Bu, Ph, Me2CHCH2, cyclohexyl, EtMeCH, CF3, thexyl) were prepd. and their ene reaction with cyclohexene, a 1,2-disubstituted ene having the least steric requirement, examd. In this reaction, a trifluoromethyl group was found to behave as if it were a much larger substituent than a Ph or iso-Bu group and as large as a sec-Bu group.
ST steric effect trifluoromethyl group ene reaction; ketone trifluoromethyl ene reaction; stereochem ene reaction trifluoromethyl ketone; regiochem ene reaction trifluoromethyl ketone
IT Steric effect
(of trifluoromethyl group on ene reaction of trifluoromethyl ketones)
IT Trifluoromethyl group
(steric effect of, on ene reactions of trifluoromethyl ketones)
IT Addition reaction
(ene, of trifluoromethyl ketones, steric effect of trifluoromethyl group on)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(trifluoromethyl, ene reaction of, steric effect of trifluoromethyl group on)
IT 76-05-1, Trifluoroacetic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of)
IT 108-85-0, Cyclohexyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with iso-Bu trifluoromethyl ketone)
IT 78-77-3, Isobutyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetic acid)
IT 1521-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with trifluoroacetophenone)
IT 75-90-1, Trifluoroacetaldehyde 360-34-9 421-50-1 434-45-7, .alpha.,.alpha.,.alpha.-Trifluoroacetophenone 684-16-2, Hexafluoroacetone
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, steric effect of the trifluoromethyl group in)
IT 433-27-2, Trifluoroacetaldehyde ethyl hemiacetal
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with dimethylbutenes)
IT 563-79-1, 2,3-Dimethyl-2-butene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with trifluoroacetaldehyde)
IT 110-83-8, Cyclohexene, reactions 13389-42-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with trifluoromethyl ketones)

IT 116356-54-8P 122129-36-6P 122129-38-8P 141779-27-3P 141779-28-4P
141779-29-5P 141779-30-8P 141779-31-9P **141779-32-0P**
141779-33-1P **141779-34-2P 141779-35-3P** 141779-36-4P
**141779-37-5P 141779-38-6P 141779-39-7P**
141779-42-2P 141779-43-3P 141779-44-4P 141846-75-5P 141846-76-6P
141846-77-7P 141899-03-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)

IT 114420-54-1P 122129-28-6P 122129-29-7P 122129-30-0P 122129-31-1P
125458-29-9P 134166-51-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 134166-52-2P 134166-53-3P 134166-54-4P 134166-55-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and dehydration of)

IT 6302-04-1P, Cyclohexyl trifluoromethyl ketone 75703-02-5P, Isobutyl trifluoromethyl ketone 134166-49-7P, sec-Butyl trifluoromethyl ketone 134166-50-0P, Thexyl trifluoromethyl ketone
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and ene reaction of, steric effect of the trifluoromethyl group in)

IT 141779-40-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and hydrogenation of)

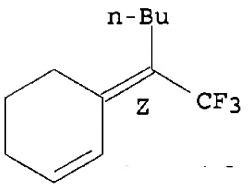
IT 141779-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., spectra and oxidn. of)

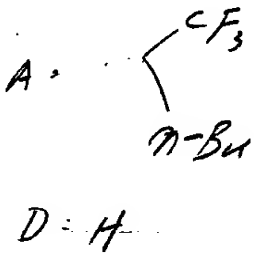
IT **141779-32-0P 141779-34-2P 141779-35-3P**
**141779-37-5P 141779-38-6P 141779-39-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)

RN 141779-32-0 CAPLUS

CN Cyclohexene, 3-[1-(trifluoromethyl)pentylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

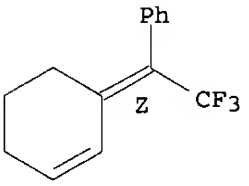


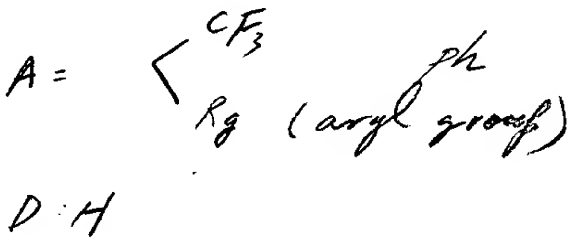




RN 141779-34-2 CAPLUS

CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



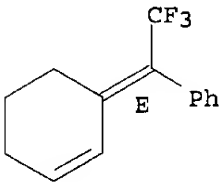




RN 141779-35-3 CAPLUS

CN Benzene, [1-(2-cyclohexen-1-ylidene)-2,2,2-trifluoroethyl]-, (E)- (9CI)

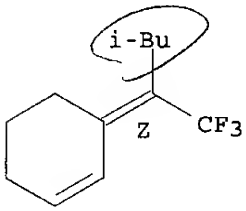
(CA INDEX NAME)

Double bond geometry as shown.



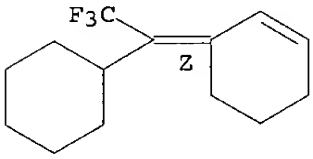

RN 141779-37-5 CAPLUS
CN Cyclohexene, 3-[3-methyl-1-(trifluoromethyl)butylidene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.




RN 141779-38-6 CAPLUS
CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.




RN 141779-39-7 CAPLUS
CN Cyclohexene, 3-(1-cyclohexyl-2,2,2-trifluoroethylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.